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Data Article

Prediction of the properties of eutectic organic phase change materials

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ABSTRACT

The data presented in this article include the molar masses, melting temperatures, latent heats of fusion and temperature-dependent heat capacities of fifteen fatty acid phase change materials (PCMs). The data are used in conjunction with the thermodynamic models discussed in Kahwaji and White (2017) to develop a computational tool that calculates the eutectic compositions and thermal properties of eutectic mixtures of PCMs. The computational tool is part of this article and consists of a Microsoft Excel® file available in Mendeley Data repository, http://dx.doi.org/10.17632/243d6r4z26.1. A description of the computational tool along with the properties of nearly 100 binary mixtures of fatty acid PCMs calculated using this tool are also included in the present article. The Excel® file is designed such that it can be easily modified or expanded by users to calculate the properties of eutectic mixtures of other classes of PCMs.

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Specifications Table

Subject area	*Thermal energy storage*
More specific subject area	*Phase change materials (PCMs), Eutectic mixtures of PCMs*
Type of data	*Table, Microsoft Excel® file*
How data were acquired	*Differential scanning calorimetry (DSC) using a TA Instrument Q200 DSC, published literature*
Data format	*Raw, analyzed*
Experimental factors	*PCM samples measured as acquired from suppliers*
Experimental features	*A combination of measured and published data is used to calculate the properties of new PCMs formed from binary eutectic mixtures.*
Data source location	*Not applicable*
Data accessibility	*Data are available in this article and the Excel® file is available from [mawhite.chem.dal.ca/Eutectic_Mixtures_Workbook.xlsm]*

Value of the data

- The data include the melting temperatures, T_{mpt}, latent heats of fusion, $\Delta_{fus}H$, and heat capacities, $C_p(T)$, of 15 fatty acid PCMs and the eutectic composition, T_{mpt} and $\Delta_{fus}H$ of 97 eutectic PCMs.
- The data allow the selection of an appropriate PCM for thermal energy storage applications in a wide temperature range, from − 22 to 75 °C.
- The data are included as a default database in the provided Excel® file. The Excel® file can be used to predict which binary mixture yields a user-specified melting temperature.
- The dataset in the Excel® file can be edited by researchers to include their own measured values of thermal properties, for a more accurate prediction of the properties of eutectic PCMs.
- Researchers also can expand the dataset of the Excel® file, *e.g.*, to include the properties of another class of PCMs and find their eutectic mixtures, or use the calculated values to determine the properties of higher order (*i.e.*, ternary or quaternary) mixtures of PCMs.

1. Data

The data presented in this article include the molar masses and thermal properties of 15 fatty acid PCMs (Table 1). The thermal properties are the melting temperature, T_{mpt}, the latent heat of fusion, $\Delta_{fus}H$, and the heat capacities as a function of temperature, $C_p(T)$, for both the solid and liquid phases. We measured T_{mpt}, $\Delta_{fus}H$ and $C_p(T)$ of five fatty acids: decanoic acid (C10 thereafter), dodecanoic acid (C12), tetradecanoic acid (C14), hexadecanoic acid (C16) and octadecanoic acid (C18) by DSC [1], whereas for the other fatty acids, the values of T_{mpt}, $\Delta_{fus}H$ and $C_p(T)$ were obtained from the literature [2,3]. The data in Table 1 are the basis of the Excel® file, available from the following link: http://dx.doi.org/10.17632/243d6r4z26.1. The Excel® file contains equations from the thermodynamic models discussed in the manuscript entitled "*Prediction of the Properties of Eutectic Fatty Acid Phase Change Materials*" (Kahwaji and White, 2017) and was used to compute the eutectic compositions and thermal properties of all 105 possible binary combinations of the fatty acid PCMs. A total of 97 combinations form binary eutectic mixtures and their properties are included in Tables 2–5, presented according to the range of the eutectic temperature, T_{eut}, of the mixtures.

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